Template for highest materials modelling metadata

1. The properties and behaviour of the material: nanoparticle size distribution, morphology and internal composition via modelling of the synthesis process from gas phase condensation, including homogeneous and heterogeneous nucleation, surface and internal chemical kinetics and composition, agglomeration, aggregation.
2. Chain of models calculating these properties and behaviour: MD, CG-MD and fluid mechanics.

Atomistic Model

1. **Generic physics of the model equation**
   Classical Molecular Dynamics
   1.1. This is a materials model for atoms
   1.2. The model contains the Newton's equation of motions involving position, velocity, mass, interatomic forces and closure relations that are: ReaxFF reactive interatomic potentials which involves positions and interatomic forces and thermostat (e.g. Langevin) which involves statistical thermodynamics (temperature, pressure, volume).

2. **End-user problem/system that is simulated (type of metadata: declarations)**
   This is the "model application", "case to be studied".
   2.1. Specify material properties, behaviour and/or material manufacturing processes simulated. nucleation of atoms from gas phase to form primary nanoparticles, surface condensation, nanoparticle reactive interaction with gas species, mutual interaction between nanoparticles (i.e. agglomeration, sintering) Si, ZnO, Al_3O_3, Pt in $Ar/H_2/N_2/O_2$ atmospheres in plasma, hot wall and flame nanoparticle synthesis processes
   2.2. Size, form, geometry, picture of the system and time lapse of the process
   nanometer sized cubic box, femtoseconds
   2.3. Physics metadata for system that is simulated. Here should be listed
   - physics quantities that do not appear in the physics equation and not in the case description above but that are relevant to describe the system/problem/ model application/case like e.g. density, external pressure, viscosity, chemical composition, impurities, mobility: density of condensing species (Si, ZnO, Al_2O_3, Pt), temperature time gradient, Knudsen number (diffusion or free molecular regime), chemical composition.
   - process conditions (like heated walls, external pressures, bending forces) to be simulated): temperature time gradient (cooling), fixed pressure

   (Note this should not describe the output!)
   2.4 Publication documenting the simulated case: <future project publications will be listed>

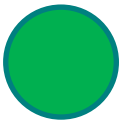
3. **Computational modelling metadata for the case that is simulated (type of metadata: values/data)**
   3.1 Numerical Solver: Verlet-type algorithm for Newton's dynamics

3.2 Input you need to start computing, e.g. times step, number of “fictitious” particles (only in case this can be chosen freely like in Lagrangian solvers), grid size, computational boundary conditions, “fictitious” particle positions and velocities (that you can choose freely but are necessary to start computing).

Type of Input: species number densities, volume and temperature evolution in time for the thermostat, time step, size of the simulation box that will be replicated, ReaxFF force field parameters

Boundary conditions: periodic

3.3 Initialisation of all quantities and parameters (appearing in Ch1, Ch2, Ch3.1): (these are the code's input files and can for the moment remain empty until uploaded into a repository) random atom positions (or already assembled in nanoparticles), Maxwellian based random velocity distribution



3.4 Keywords describing “raw output” calculated by the model for the entities: Atoms position as function of time calculated by the model for the atomic species

3.5 Keywords for “post processed properties” calculated for atoms from the raw output calculated with self-developed data analysers to identify and extract mesoscopic entities (e.g. primary particles) and quantities such as: homogeneous nucleation rate, heterogeneous nucleation rate, nanoparticle size distribution, nanoparticle interaction potential, nanoparticle surface reaction rates, nanoparticles sintering time with as post processor a mapping matrix from a set of atomic coordinates to a unique nanoparticle configuration in the CG system, iterative Boltzmann conversion and/or force mapping to define CG energy functions (interparticle potential) from the atomistic ones.

3.6 Margin of error of property calculated under 3.3: accuracy of ReaxFF parameters, application on limited time and domain and to one mechanisms at time (i.e. sintering, nucleation), multiparticle interactions are often neglected in favour of binary interaction.

3.7 Publication documenting the simulation

Mesoscopic Model

1. **Generic physics of the model equation**

   Coarse Grained Molecular Dynamics

   1.1. This is a materials model for grains (nanoparticles)

   1.2. The model contains

   - the Newton's equation of motions (solved by Montecarlo and/or population balanced methods) for each nanoparticle involving position, velocity, mass, nanoparticle interaction forces and closure relation that expressed the nanoparticle interaction forces between grains (nanoparticles) based on van der Waals potentials, which involves homogeneous nucleation rate, heterogeneous nucleation rate, nanoparticle size distribution, particle surface and internal reaction rates.
   - the equation for the evolution in time of the common surface between two nanoparticle involving temperature, particle diameters and characteristic sintering time and closure relation that involve material dependent sintering parameters
   - species conservation equations of each nanoparticle (including chemical kinetics and heterogeneous nucleation) involving temperature, gas phase and nanoparticle species concentration, surface reaction rates, surface condensation rate and closure relation that involve gas phase and nanoparticle species concentration and temperature based on reaction rate coefficients and classical nucleation theory

   1.3 Publication documenting the above

2. **End-user problem/system that is simulated (type of metadata: declarations)**

   This is the "model application", "case to be studied".

   2.1 Specify material properties, behaviour and/or material manufacturing processes simulated. nanoparticle formation in a fluid volume and evolution of the nanoparticle ensemble including agglomeration, sintering and chemical reactions

   Si, ZnO, Al_3O_3, Pt in $Ar/H_2/N_2/O_2$ atmospheres in plasma, hot wall and flame nanoparticle synthesis processes

   2.2 Size, form, geometry, picture of the system and time lapse of the process

   micrometer sized cubic box, milliseconds

   2.3 Physics metadata for system that is simulated. Here should be listed:

   - physics quantities that do not appear in the physics equation and not in the case description above but that are relevant to describe the system/problem/model application/case like e.g. density, external pressure, viscosity, chemical composition, impurities, mobility:

     The same as the atomistic model, since physical phenomena are the same, but described with different model approaches: density of condensing species (Si, ZnO, Al_2O_3, Pt), temperature time gradient, Knudsen number (diffusion or free molecular regime), chemical composition.
   - process conditions (like heated walls, external pressures, bending forces) to be simulated): temperature time gradient (cooling), fixed pressure.

   2.4 Publication documenting the simulated case

3 **Computational modelling metadata for the case that is simulated**

3.1 Numerical Solver: Verlet-type algorithm for simulating Langevin dynamics, newton like solver for chemical kinetics equations.

3.2 Input you need to start computing, e.g. times step, number of “fictitious” particles (only in case this can be chosen freely like in Lagrangian solvers), grid size, computational boundary conditions, “fictitious” particle positions and velocities (that you can choose freely but are necessary to start computing).

Type of Input: volume, gas phase species number densities and temperature evolution in time, homogeneous nucleation rate, heterogeneous nucleation rate, nanoparticle size distribution, nanoparticle interaction potential, nanoparticle surface reaction rates, nanoparticles sintering time, chemical kinetics coefficients; random initial particle positions depending on temperature

Boundary conditions: periodic

3.3 Initialisation of all quantities and parameters (appearing in Ch1, Ch2, Ch3.1): (these are the code's input files and can for the moment remain empty until uploaded into a repository)

3.4 Keywords describing “raw output” calculated by the model for the entities: : positions, aggregates and agglomerate structures calculated by the model for the entities grains (nanoparticles)

3.5 Keywords for “post processed properties” calculated for grains from the raw output calculated with self-developed mesoscopic model dataset analysers:

morphology and size of aggregates and agglomerates (e.g. fractal dimension), nanoparticles size distribution, nanoparticles composition, nanoparticles morphology calculated for grains (nanoparticles)

Post-processor: simple integration on the particle set or particle counting

precursor vapour consumption for continuum model coupling

storage of the homogeneous and homogeneous nucleation rates per time step

3.6 Margin of error of property calculated under 3.3: errors related to particle idealization (e.g. spherical shape), chemical reduction, interparticle forces, sintering mechanism and limited number of particles in the mesoscopic ensemble. Also using temperature and composition data from a continuum fluid model streamline nanoparticle diffusion is neglected.

3.7 Publication documenting the simulation

Continuum models

1. **Generic physics of the model equation**

   Fluid Dynamics

1.1. This is a materials model for finite volumes

1.2. The continuum model contains continuum equations that describe fluid dynamics, heat transfer, turbulence, species diffusion that describe non-equilibrium chemistry, combustion, plasma MHD, transport of the gas phase precursor vapours and well-established closures relations that involves all the typical continuum quantities (e.g. velocity, density, species concentration) such as the Newtonian linear relationship between stress and deformation tensors in Navier-Stokes equation, RANS models closures for turbulent stress tensors (e.g. k-ε, k-ω) or the Fourier law for heat conduction.

2. **End-user problem/system that is simulated (type of metadata: declarations)**

   This is the "model application", "case to be studied".

   2.1. Specify material properties, behaviour and/or material manufacturing processes simulated

   Flow characteristics (e.g. velocity, temperature, species concentration) in a gas phase reactors (plasma, flame and hot wall reactors) Si, ZnO, Al_3O_3, Pt in $Ar/H_2/N_2/O_2$ atmospheres in plasma, hot wall and flame nanoparticle synthesis processes

   2.2. Size, form, geometry, picture of the system and time lapse of the process

   centimetres, seconds

   2.3. Physics metadata for system that is simulated. Here should be listed

   - physics quantities that do not appear in the physics equation and not in the case description above but that are relevant to describe the system/problem/ model application/case: gas composition, turbulent viscosity.
   - process conditions (like heated walls, external pressures, bending forces) to be simulated): gas heating by combustion, plasma or heated wall; gaseous, liquid or solid precursors; controlled temperature evolution; fixed pressure

   2.4 Publication documenting the simulated case:

3. Computational modelling metadata for the case that is simulated (type of metadata: values/data)

3.1 Numerical Solver: Finite volume (GS based algebraic multigrid)

3.2 Input you need to start computing, e.g. times step, number of "fictitious" particles (only in case this can be chosen freely like in Lagrangian solvers), grid size, computational boundary conditions, "fictitious" particle positions and velocities (that you can choose freely but are necessary to start computing).

Type of Input: process operating conditions, reactor geometry and type, species condensation rate (i.e. gas phase to nanoparticles).

Boundary conditions: reactor dependant, based on user defined operating conditions user inputs

3.3 Initialisation of all quantities and parameters (appearing in Ch1, Ch2, Ch3.1): (these are the code's input files and can for the moment remain empty until uploaded into a repository)

3.4 Keywords describing “raw output” calculated by the model for the entities
flow fields, temperature fields, species concentrations calculated by the model for the finite volumes (gas phase).

3.5 Keywords for “post processed properties” calculated for finite volumes from the raw output calculated with generic CFD post-processing (e.g. paraview): position in time (i.e. streamline), temperature in time, species concentration in time calculated for single finite volume.

3.6 Margin of error of property calculated under 3.3: error related to the limited amount of streamline used for mesoscopic models, chemical reduction, turbulence models.

3.7 Publication documenting the simulation: V Colombo, E Ghedini, M Gherardi and P Sanibondi, “Modelling for the optimization of the reaction chamber in silicon nanoparticle synthesis by a radio-frequency induction thermal plasma”, *Plasma Sources Sci. Technol.* 21 (2012) 055007 (10pp)